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Development of Mathematical Model for Balance Settlement of Product and Waste Flows from SNF Reprocessing

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Abstract

A mathematical model has been built to estimate steady-state characteristics of flows and products in SNF processing systems. A developed calculation module will enable to change not only a type of SNF to be reprocessed and relationship among the processing units (stages) while building the model, but also will provide for entering new processing stages into the model to develop new process flow-sheets, to optimize and to compare the existing ones. Optimizing calculations have been conducted on the basis of the model regarding new promising flow-sheets of reprocessing SNF from fast reactors. The selected data structure within the model will provide for modelling of not only SNF reprocessing but also of other nuclear fuel processing stages.

Keywords: mathematical model, process flow sheets, calculation modules.

1. Introduction

Model-building aspect including nuclear fuel cycle and transportation has to become a most important section under a large-scale nuclear energy program development. It is only on the basis of perfect models of nuclear energy and nuclear fuel cycle that the neutral balance in the system and nuclear flows of nuclear materials (nuclear logistics) can be optimized and controlled. Model building will allow to realize an integrated system analysis of the waste handling (transportation, separation, transmutation, temporary storage, disposal within geological formations) and to substantiate safety of the nuclear fuel cycle.

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2. Review of the existing models

Reprocessing of SNF from the nuclear power plants is an important element of the closed nuclear fuel cycle. The start of new flowsheet development or existing flowhseet modernization is preliminary estimation of main parameters of studied flowshheet. First step of flowsheets investigation is a calculation of nuclides logistic inside of the flowsheet. It is a absolutely necessary step. Thus it ia a necessary to develop a mathematic model which will be able to made a calculation of nuclide logistic and easy change the flowsheet and composition treated nuclear fuel. Currently, there many models to describe nuclear fuel cycle as a whole and individual parts or technologies thereof. The following ones can be identified as the most popular models: VISTA [1], ATEK [2], Prognosis [3], Message [4], DESAE[4] etc.

The above-mentioned models are software complexes consisting of units to correspond to various stages of the nuclear fuel cycle (NFC). Such models as VISTA, Message, DESAE can be used for estimation of longtime strategy of regional or international nuclear cycle. The main advantage of VISTnA, Message and DESAE models is a calculation of all system as whole. For example Vista allows us to change a number of parameters (type of reactor, open or closed nuclear fuel cycle, duration of calculated period. The amount of needed uranium, fresh and spent nuclear fuel and etc. are the main results of calculation. The friendly interface and low calculation time are the advantages of this model. However the model VISTA is makes a calculation only as results of several parts of nuclear fuel cycle and does not calculated the nuclides logistic inside of the parts. Models ATEK and Prognosis have the same advantages and aims as a VISTA. There is a possibility to calculated the nuclides logistic inside of several parts of nuclear fuel cycle using models ATEK or Prognosis. However the flowsheet of nuclides logistic inside of nuclear fuel parts are fixed for these models, because these model use the real existing flosheets, for example PUREX-process for reprocessing. It is necessary to add that only authors can change the flosheet inside these models.

Considering that many technologies are still not entirely settled and allow for alterations in interrelations among themselves or variations in technological choice, a model is necessary that will also tolerate adjustments in the analytical model applied by a user when working the software complex.

3. Problem Definition

As it was mentioned above the main peculiarity of our model is a ability to collect a flowsheet using the separate elements and make a connection between them. The possibility to alter the relations among flowsheet elements results in the situation when it is not feasible to consider SNF-reprocessing as a single object when building a model. Thus it is sensible to use the basics of system-modelling [5, 6], according to which a complex system has be divided into simpler parts with relation among the latter to be set.

In our case the elements of the complex system may be units used in SNF-reprocessing or groups of such units if the relations within the groups are not to be altered while the relations among the groups will be flows of material substances. In this case each of the units incorporated into the system must have a related model that allows identifying parameters of out-coming flow depending on parameters of the incoming one. Integration of the unit models should be in accordance with the flow sheet set by a user. Thus, model building for the balance flow modelling for the SNF-reprocessing has to include the stages as follows:

- Formalizing of the dated used in the model
- Creation of a user-interface to enter bench marks and plotting calculation results
- Development of algorithms for a model according to a user flow-sheet
- Creation of models of units used in SNF-reprocessing.

4. Data Structure

One of the requirements for the developed model has been to allow the model to be used not only by its designers. Thus there appeared a necessity to create a full-fledged computer software. To develop the software an object-oriented programming language c# [7] has been chosen. The main advantage of the language is a clear observance of the basic principles of the object-oriented coding (OOC) in addition to ease of user interface creation [8]. The main advantage of the OOC is a possibility to consider the system to be simulated as a complex of objects. There are three major type of objects in the task we are dealing with (classes according to the OOC) – unit, flow, flow-sheet.

The class 'flow' consists of a number of chemical components consisting, in turn, of a number of chemical elements, and it has the features as qualities: state of matter, specific gravity, velocity (mass unit per time unit). So a flow of velocity of 1 standard unit of 1m solution of nitric acid will include two components: water and nitric acid, each of which has its own element composition (fig.1).

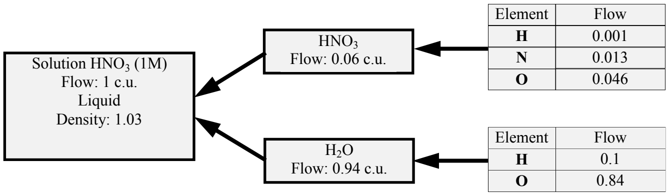


Figure 1 – diagram of the data structure within the class 'Flow'

The class 'Unit' (Fig. 2) includes a model of the system element (unit, process, block of units). The main function of the class elements is to transform the flows coming into the unit into the flows coming out of the unit. The main content of this class is a method contained therein that transforms incoming flows and that is unique for each type of the units included in the system to be modelled. In addition to the flow transformation method this class consists of modelling methods for reagents required for the process, assessments of quality of the process being modelled and may consist of the most important characteristics of the process.

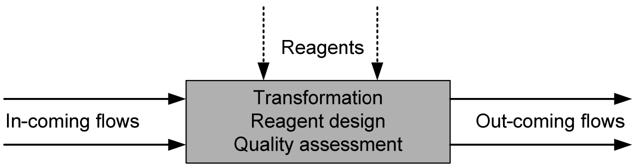


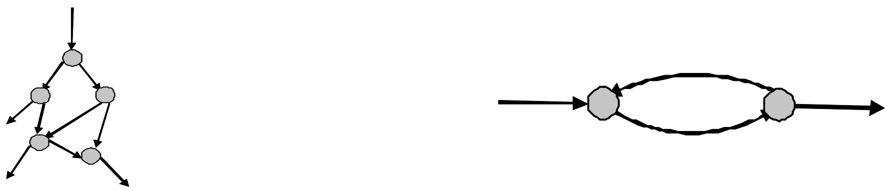
Figure 2 – Diagram of the unit class

The function of class 'Flow-sheet' is collecting of all the bench marks required for calculations. An object of this class consists of a number of units comprising the flow-sheet, an array o flows among the units and interface conditions for the flow-sheet in question, i.e. the flows that do not come out of any part of the flow-sheet. As the bench marks have to be set by a user this object in contrast to any other has an interface lowing for the user to set up a flow-sheet and interface conditions and a method of transition of the data set by the user into the data accepted for the calculations. Availability of all the information on the flow-sheet under modelling (the interface conditions used for designing of the units and integration layout thereof) allows for calculations based on the data set by the user via the calculation block in the software.

5. Calculation module

The software under review consists of three main parts: unit to enter the scheme, the calculation module and block of results visualization. The first and last blocks are needed to translate computer representation of data into a clear and user-friendly look. Interaction between the user and the calculation module is not directly implemented. The function of the calculation module according to the user set data is to determine the characteristics of all the flows within the circuit. Searching of flow characteristics is carried out via combination of several mathematical methods based on graph theory [9] and the numerical and analytical methods for solving algebraic equations.

A user begins solving the problem with an analysis of the system, which is required to determine the sequence of methods to be used. The whole flow-sheet can be divided into two types of blocks, computation of which is carried out in different ways. Figure 3 shows variations of these types of diagram blocks as a set of units and flows. A characteristic feature of the dendrogram is that one can always choose a sequence of units so that with calculation of flows using each subsequent unit the flows incoming into this unit will be known. In other words the calculation is performed sequentially in this scheme during the transition from unit to unit. In this case, the problem of finding all the characteristics of the flow reduces to finding the execution order for transformations that can be easily solved if one relies on the known solutions of problems in graph theory [9]. In contrast to a dendrogram a cyclic pattern does not have a sequence of operations that would allow to perform calculation based on transition from one unit to another. That is because at least one flow coming into a certain unit in such a flow-sheet depends on the flow coming out of the same unit. Thus other calculation methods are required for this type of flow-sheet.



dendrogram cyclic

Figure 3 – typical flow-sheet blocks.

Since it is impossible to calculate flows with consistent transformation inherent in the units in the case of cyclic patterns, all the transformations and flows should be considered together. Because each thread is determined by a dependence on the values of all other flows in the circuit, a cyclic pattern can be associated with a system of algebraic equations, in which variables are the flow values. A difficulty in solving such a system is that conversion are not known in the units in advance, which results in the need to solve the system in general terms by numerical methods.

Analysis of existing numerical methods for solving systems of algebraic equations [10] shows that one of the iterative solution methods, modified by taking into account the features of the problem, should be used The analysis of the problem being solved and the modification of existing algorithms have resulted in the following algorithm for flow calculation in a cyclic pattern. The first step sets the values of all unknown flows in the circuit (zero iteration). The second step is the calculation of the flows in random order (first iteration), and the values of the flows coming into the unit are known and given by the previous iteration. We compare the calculated flows with the values corresponding to the previous iteration. If the value difference is small, the latter option is a designed solution to the problem of finding the flows in a cyclic pattern. If the difference is essential, it is calculated similar to the one described in the second step, and the results are compared with the previous calculation. The operation is repeated until one reaches the required accuracy of the calculation.

Obviously, quite complex patterns that occur in SNF-reprocessing can not be ranked according to one the listed types, but they can be divided into blocks corresponding to such flow-sheets. So the first step in calculating a user-defined problem should be division of the whole flow-sheet into blocks with the same type of communication between units. The solution is based on the graph theory [9]. In the whole scheme, cycles are to be determined and all other elements of the flow-sheet should be included into the dendrogram-type blocks of the flow-sheets using the goals and tenets of this theory. Calculating sequence should be determined for the blocks, then the calculation is performed in each block according to the algorithms described above.

6. Conclusion

A mathematical model has been built to estimate steady-state characteristics of flows in the SNF-reprocessing flow-sheets. The model is developed as a computer application that allows for a wide range of users to use the model. The main part of the model is the calculation module, which performs an analysis of the simulated circuit and automatically selects the mathematical method of calculation. Due to the developed calculation module it is possible to change the composition of the flow-sheet and links between processes in the scheme when building a model. That is its undoubted advantage in development of new flow-sheets of the process and in comparing different versions of technological flow-sheets. Optimizing calculations have been conducted on the basis of the model with regard to the new promising flow-sheets of SNF-reprocessing for fast reactors with liquid-metal coolant. Due to the fact that the model is divided into independent modules, it can be used in the simulation of both whole plants and individual operations. The developed data structure within the computer application makes it easy to add new database models and existing models with new data.

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